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LETTER TO THE EDITOR

Non-spurious two-cluster harmonic oscillator wavefunctions

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Abstract. We consider a system of identical particles distributed in two clusters and described by harmonic oscillator wavefunctions. A set of non-spurious two-cluster states, whose centre-of-mass is at rest, is constructed. It is characterized by the cluster Yamanouchi symbols as well as by its overall permutational symmetry, angular momentum and total energy. Applications to nuclear cluster models, to the evaluation of nuclear spectroscopic factors, to the description of nuclei as quark-clusters, and to the study of interacting rare-gas clusters are pointed out.

One of the technical difficulties that has to be faced in the study of finite systems of identical particles involves the construction of a basis set in which the spurious centre-of-mass motion is excluded. One common procedure involves the construction of a basis set contaminated by spurious states, which have then to be eliminated. This is usually done by adding an appropriate interaction to the Hamiltonian which pushes up the spurious states in such a way that they do not affect the eventual calculations [1]. However, these states are still present, yielding large, inefficient basis sets.

An explicit elimination of the centre-of-mass can be achieved by using a harmonic oscillator basis set in Jacobi coordinates. The use of this approach for the construction of non-spurious nuclear wavefunctions was studied extensively by Kramer and Moshinsky [2, 3] and, in a different manner, by Smirnov *et al* [4, 5] and by Vanagas [6]. A detailed exposition of these applications is presented by Wildermuth and Tang [7].

A new approach for constructing single-cluster harmonic oscillator (HO) wavefunctions with arbitrary permutational symmetry was recently proposed [8]. In this approach the HO wavefunction is separated into an internal wavefunction in terms of $n-1$ Jacobi coordinates and a centre-of-mass wavefunction. The internal states are constructed recursively using a new type of HO coefficients of fractional parentage (HOCFPS). Keeping the centre-of-mass at rest we obtain a basis set consisting of non-spurious HO states.

A more serious difficulty is encountered in the calculation of spectroscopic factors in nuclear reactions [4, 5]. These involve non-spurious two-cluster HO wavefunctions. Several methods have been proposed to eliminate two-cluster spurious states, but each one of them is only applicable within a small class of special cases [1].

In the present letter we introduce a general procedure to construct non-spurious two-cluster states with arbitrary permutational symmetry. The two-cluster states are expressed in terms of two single-cluster internal wavefunctions coupled to a HO relative wavefunction. The centre-of-mass is assumed to be at rest (0s state). Consequently,

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the overall angular momentum is the same as the internal angular momentum. In addition, the centre-of-mass wavefunction is totally symmetric with respect to permutations of the particle coordinates and therefore does not affect the overall permutational symmetry. In view of the above, we will consider only the internal wavefunction.

For a single cluster of n identical particles, the sequence of irreducible representations (irreps) $\Gamma_{[2]}, \Gamma_{[3]} \ldots \Gamma_{[n-1]}, \Gamma_{[n]}$ of the permutation group–subgroup chain $S_{[2]} \subset S_{[3]} \subset \ldots \subset S_{[n-1]} \subset S_{[n]}$ completely determines the permutational symmetry of the wavefunction. This sequence of irreps is equivalent to a Yamanouchi symbol $Y_{[n]}$. Therefore, the internal wavefunction of an n-particle single cluster with a well defined permutational symmetry is [9]

$$|Y_{[n]}\Phi_{[n]}; \boldsymbol{\rho}_{\{2\},[1]}\boldsymbol{\rho}_{\{3\},[2]} \cdots \boldsymbol{\rho}_{\{n\},[n-1]}\rangle \tag{1}$$

where $[n] \equiv \{1, 2, \ldots, n\}$. The symbol $\Phi_{[n]}$ denotes the remaining good quantum numbers

$$\Phi_{[n]} = \Lambda_{[n]}\varepsilon_{[n]}\alpha_{[n]} \tag{2}$$

where $\Lambda_{[n]}$ is the overall internal angular momentum, $\varepsilon_{[n]}$ is the total internal energy and $\alpha_{[n]}$ is an additional label that takes care of any remaining degeneracy.

The wavefunction (1) is expressed in terms of the $n-1$ Jacobi coordinates

$$\boldsymbol{\rho}_{\{i\},[i-1]} = \left(\boldsymbol{r}_i - \frac{\boldsymbol{r}_1 + \boldsymbol{r}_2 + \ldots + \boldsymbol{r}_{i-1}}{i-1}\right)\sqrt{\frac{i-1}{i}} \tag{3}$$

where $i = 2, 3, \ldots, n$. This set of coordinates was found to be convenient because each internal coordinate $\boldsymbol{\rho}_{\{i\},[i-1]}$ depends on the first i single particle coordinates only. This property enables the formulation of a recursive procedure for constructing the states specified by (1), as presented in [8].

We now consider two-cluster HO states. The particles are distributed in these two clusters in such a way that there are n_1 particles in one cluster and n_2 particles in the other, where $n_1 + n_2 = n$. The good quantum numbers of a two-cluster wavefunction are the Yamanouchi symbols of the two clusters, $Y_{[n_1]}$ and $Y_{[n_2]'}$, the total permutational irrep symbol $\Gamma_{[n]}$, angular momentum $\mathscr{L}_{[n]}$ and internal energy $\varepsilon_{[n]}$ (cf [10]). The symbol $[n_1]$ stands for the particle indices in the first cluster, $[n_2]'$ for the indices in the second, and $[n] = [n_1] \cup [n_2]'$. The two-cluster wavefunction is constructed in terms of a basis set consisting of states of the form

$$|(Y_{[n_1]}\Phi_{[n_1]}Y_{[n_2]'}\Phi_{[n_2]'})\Lambda_{[n]}\Phi_{[n_2]',[n_1]}\mathscr{L}_{[n]}\varepsilon_{[n]}\rangle. \tag{4}$$

The intercluster HO wavefunction

$$|\Phi_{[n_2]',[n_1]}\rangle = |N_{[n_2]',[n_1]}L_{[n_1][n_2]'}; \boldsymbol{\rho}_{[n_2]',[n_1]}\rangle \tag{5}$$

is expressed in terms of the intercluster relative coordinate

$$\boldsymbol{\rho}_{[n_2]',[n_1]} = \left(\frac{\boldsymbol{r}'_1 + \boldsymbol{r}'_2 + \ldots + \boldsymbol{r}'_{n_2}}{n_2} - \frac{\boldsymbol{r}_1 + \boldsymbol{r}_2 + \ldots + \boldsymbol{r}_{n_1}}{n_1}\right)\sqrt{\frac{n_1 n_2}{n_1 + n_2}}. \tag{6}$$

$N_{[n_2]',[n_1]}$ and $L_{[n_2]',[n_1]}$ are the corresponding radial and angular quantum numbers.

The total internal energy is

$$\varepsilon_{[n]} = \varepsilon_{[n_1]} + \varepsilon_{[n_2]'} + \varepsilon_{[n_2]',[n_1]} \tag{7}$$

where

$$\varepsilon_{[n_2]',[n_1]} = 2N_{[n_2]',[n_1]} + L_{[n_2]',[n_1]} + \tfrac{3}{2} \tag{8}$$

is the internal energy associated with the intercluster relative motion. The angular momenta are coupled in the two-cluster states (4) in the following order: first we couple the angular momenta of the two clusters $\Lambda_{[n_1]}+\Lambda_{[n_2]}=\Lambda_{[n]}$ and then we couple the resultant angular momentum with the angular momentum of the intercluster relative motion. This yields the overall internal angular momentum, i.e. $\Lambda_{[n]}+L_{[n_2]',[n_1]}=\mathscr{L}_{[n]}$.

The states (4) do not have a well defined n-particle permutational symmetry. Our aim in the present letter is to show how to construct a set of states which, in addition to the good quantum numbers mentioned above (i.e. the Yamanouchi symbol of each cluster, the total energy and angular momentum) can be labelled in terms of their overall permutational symmetry.

A method to construct multicluster wavefunctions with well defined permutational symmetry in an arbitrary single particle basis was recently developed [10]. An appropriate set of class-operators of the symmetric group [11] is diagonalized within the subspace of multicluster states with a given choice of single-cluster Yamanouchi symbols and a given total angular momentum. The common eigenstates of these class-operators belong to irreps of the symmetric group that are fully specified by the corresponding eigenvalues. The resulting states contain the spurious centre-of-mass motion in an uncontrolled and inseparable way.

A very similar procedure can be adopted to the present context. Since the functions given by (4) are non-spurious, so will be any linear combination of such functions. Choosing any desirable values for $Y_{[n_1]}$, $Y_{[n_2]'}$, $\mathscr{L}_{[n]}$ and $\varepsilon_{[n]}$, and noting that the corresponding operators commute with the class-operators of the symmetric group $S_{[n]}$, we diagonalize the latter and obtain linear combinations belonging to irreps denoted by $\Gamma_{[n]}$

$$
\begin{aligned}
&|(Y_{[n_1]}Y_{[n_2]'})\Gamma_{[n]}\mathscr{L}_{[n]}\varepsilon_{[n]}\alpha_{[n]}\rangle \\
&\quad=\sum_{\Phi_{[n_1]}\Phi_{[n_2]'}\Phi_{[n_2]'[n_1]}\Lambda_{[n]}}[(Y_{[n_1]}\Phi_{[n_1]}Y_{[n_2]'}\Phi_{[n_2]'})\Lambda_{[n]}\Phi_{[n_2]',[n_1]}\mathscr{L}_{[n]}\varepsilon_{[n]}| \\
&\qquad\times(Y_{[n_1]}Y_{[n_2]'})\Gamma_{[n]}\mathscr{L}_{[n]}\varepsilon_{[n]}\alpha_{[n]}] \\
&\qquad\times|(Y_{[n_1]}\Phi_{[n_1]}Y_{[n_2]'}\Phi_{[n_2]'})\Lambda_{[n]}\Phi_{[n_2]',[n_1]}\mathscr{L}_{[n]}\varepsilon_{[n]}\rangle \qquad (9)
\end{aligned}
$$

where $\alpha_{[n]}$ labels any remaining degeneracies.

The coefficients appearing on the right-hand side of (9) are written in a form reminiscent of the celebrated coefficients of fractional parentage of the atomic and molecular shell-models. They are the overlap integrals between the states defined in (4) and the permutational symmetry adapted states specified on the left-hand side of (9). They are in fact the common eigenvectors of the matrices representing the class-operators of $S_{[n]}$ in the basis set specified in (4).

In [10] it was shown that the matrix elements of the single cycle class operators, which are sufficient to determine the irreps of $S_{[n]}$, can be partitioned into intracluster and intercluster contributions. The former are trivial because the basis functions are eigenstates of the intracluster class-operators (cf (4)). The intercluster contribution was shown in the above reference to be expressible in terms of the matrix element of a single representative cycle. Thus, the term that has to be evaluated in order to obtain the matrix element of the class of transpositions involves the single transposition $(\{n_1\},\{n_2\}')$ between the last particle in the first cluster and the last particle in the second. For the three-cycles the only matrix elements that need to be considered are $(\{n_1\},\{n_1-1\},\{n_2\}')$, $(\{n_1-1\},\{n_1\},\{n_2\}')$, $(\{n_1\},\{n_2-1\}',\{n_2\}')$ and $(\{n_1\},\{n_2\}',\{n_2-1\}')$. The sum of the first two is a class-operator in the realization of S_3 in terms of the

indices $\{n_1\}$, $\{n_1-1\}$ and $\{n_2\}'$, and the sum of the last two is a similar class-operator in another realization of S_3. The extension to higher class-operators is obvious.

In order to evaluate these matrix elements we propose to transform the two-cluster wavefunctions (4) into three-cluster wavefunctions in which the particles appearing in the permutation of interest are placed in the third cluster. In the case of the transposition $(\{n_1\}, \{n_2\}')$ the third cluster consists of the two particles $\{n_1\}$ and $\{n_2\}'$.

The third cluster is formed recursively, one particle at a time. Assume that at a certain stage the first cluster consists of the particles $[n_1]=\{1, 2, \ldots, n_1\}$, the second consists of $[n_2]'=\{1, 2, \ldots, n_2\}'$ and the third consists of $[k]''=\{1, 2, \ldots, k\}''$. Say that we are now interested in moving the last particle of the first cluster into the third cluster. The coordinates involving this particle originally are its Jacobi coordinate within the first cluster, $\boldsymbol{\rho}_{\{n_1\},[n_1-1]}$ (equation (3)), as well as the coordinate of the centre-of-mass of the second cluster relative to that of the first, $\boldsymbol{\rho}_{[n_2]',[n_1]}$ (equation (6)), and the coordinate of the centre-of-mass of the third cluster relative to that of the first two

$$\boldsymbol{\rho}_{[k]'',[n_1]\cup[n_2]'}=\left(\frac{\boldsymbol{r}_1''+\boldsymbol{r}_2''+\ldots+\boldsymbol{r}_k''}{k}-\frac{\boldsymbol{r}_1+\boldsymbol{r}_2+\ldots+\boldsymbol{r}_{n_1}+\boldsymbol{r}_1'+\boldsymbol{r}_2'+\ldots+\boldsymbol{r}_{n_2}'}{n_1+n_2}\right)\times\sqrt{\frac{k(n_1+n_2)}{k+n_1+n_2}}. \tag{10}$$

After the transformations the particle originally referred to as $\{n_1\}$ is renamed $\{k+1\}''$ and it appears in an appropriate Jacobi coordinate within the third cluster as well as in the coordinate of that (augmented) cluster relative to the centre-of-mass of the (new) first and second clusters. In addition, we have to introduce a new relative coordinate between the (new) first cluster and the (unaffected) second one.

This situation is illustrated in figure 1, where the particle being transferred from the first cluster to the third is labelled in terms of its old and new labels. The locations of the various centres-of-mass involved in specifying the relevant coordinates, in both the original and modified clusters, are marked and labelled in the figure.

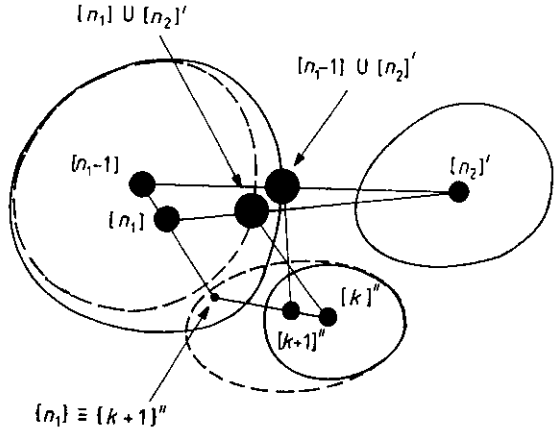

Figure 1. Transformation of a particle from the first to the third cluster. The particle transformed is $\{n_1\}$ which becomes $\{k+1\}''$. The centre-of-mass of the original clusters are at the locations labelled $[n_1]$, $[n_2]'$ and $[k]''$. Those of the new clusters are at $[n_1-1]$ and $[k+1]''$. $[n_1]\cup[n_2]'$ and $[n_1-1]\cup[n_2]'$ label the centres-of-mass of the pairs of clusters indicated.

The transformation is achieved by means of two consecutive Talmi–Moshinsky type rotations [12–14], along with appropriate angular momentum recoupling transformations which we do not specify in detail. The first rotation is

$$\begin{aligned}\boldsymbol{\rho}_{[n_2]',[n_1-1]} &= \boldsymbol{\rho}_{[n_2]',[n_1]}\cos\zeta + \boldsymbol{\rho}_{\{n_1\},[n_1-1]}\sin\zeta \\ \boldsymbol{\rho}_{\{n_1\},[n_1-1]\cup[n_2]'} &= -\boldsymbol{\rho}_{[n_2]',[n_1]}\sin\zeta + \boldsymbol{\rho}_{\{n_1\},[n_1-1]}\cos\zeta\end{aligned} \tag{11}$$

where

$$\cos\zeta = \sqrt{1-\frac{n_2}{n_1(n_1+n_2-1)}} \qquad \sin\zeta = \sqrt{\frac{n_2}{n_1(n_1+n_2-1)}}. \tag{12}$$

Note that the transformation of $\{n_1\}$ into $\{k+1\}''$ involves the identification $\boldsymbol{r}_{\{n_1\}} \equiv \boldsymbol{r}_{\{k+1\}''}$ from which it follows that $\boldsymbol{\rho}_{\{n_1\},[n_1-1]\cup[n_2]'} \equiv \boldsymbol{\rho}_{\{k+1\}'',[n_1-1]\cup[n_2]'}$. The second transformation is

$$\begin{aligned}\boldsymbol{\rho}_{\{k+1\}'',[k]''} &= \boldsymbol{\rho}_{\{k+1\}'',[n_1-1]\cup[n_2]'}\cos\eta - \boldsymbol{\rho}_{[k]'',[n_1]\cup[n_2]'}\sin\eta \\ \boldsymbol{\rho}_{[k+1]'',[n_1-1]\cup[n_2]'} &= \boldsymbol{\rho}_{\{k+1\}'',[n_1-1]\cup[n_2]'}\sin\eta + \boldsymbol{\rho}_{[k]'',[n_1]\cup[n_2]'}\cos\eta\end{aligned} \tag{13}$$

where

$$\cos\eta = \sqrt{1-\frac{n_1+n_2+k}{(n_1+n_2)(k+1)}} \qquad \sin\eta = \sqrt{\frac{n_1+n_2+k}{(n_1+n_2)(k+1)}}. \tag{14}$$

The following special cases are important.

1. The generation of the third cluster starts with the empty cluster $k=0$. In this case $\cos\eta = 0$ and $\sin\eta = 1$, i.e. $\boldsymbol{\rho}_{[1]'',[n_1-1]\cup[n_2]'} = \boldsymbol{\rho}_{\{1\}'',[n_1-1]\cup[n_2]'}$, which is obvious since $[1]'' = \{1\}''$. Thus, the second rotation (equation (13)) is superfluous.

2. Moving the last particle from the first to the third cluster. Here $\cos\zeta = 0$ and $\sin\zeta = 1$, i.e. $\boldsymbol{\rho}_{\{1\},[n_2]'} = \boldsymbol{\rho}_{[1],[n_2]'}$. In this case the first rotation (equation (11)) is superfluous.

The wavefunction for the third cluster with the additional $(k+1)''$th particle is now of the form

$$|Y_{[k]''}\Phi_{[k]''}\Phi_{\{k+1\}''}\Lambda_{[k+1]''}\varepsilon_{[k+1]''}\rangle. \tag{15}$$

Using the fact that the HOCFPS, defined in [8], form a real orthogonal matrix whose inverse is the transposed matrix, we express this state as a linear combination of the form

$$\sum_{\Gamma_{[k+1]''}}{}' [Y_{[k+1]''}\Phi_{[k+1]''}|]\,Y_{[k]''}\Phi_{[k]''}\Phi_{\{k+1\}''}\Lambda_{[k+1]''}\varepsilon_{[k+1]''}]|\,Y_{[k+1]''}\Phi_{[k+1]''}\rangle. \tag{16}$$

The prime over the summation symbol indicates that the sum is over all irreps $\Gamma_{[k+1]''}$ which are obtained by adding one box (in a legitimate position) to the irrep $\Gamma_{[k]''}$.

The transfer of a particle from the second cluster into the third one can be effected with obvious minor modifications.

Once all the relevant particles have been moved into the third cluster the evaluation of the matrix element of the intercluster class-operator becomes trivial, since the third cluster is expressed as a linear combination of terms, each one of which belongs to an irrep of the symmetric group $S_{[k]''}$. Each such term is an eigenstate of the intercluster class-operators.

The permutational symmetry adapted non-spurious two-cluster wavefunction, which we possess once the appropriate set of class-operators has been diagonalized, can be used in several very different physical contexts. It provides a very straightforward means for the evaluation of nuclear spectroscopic factors and enables the study of interacting clusters of identical particles ranging from quarks through nucleons to rare-gas atoms. Among the many applications we find the study of fission and fusion of clusters of nuclei or atoms particularly exciting. The latter are crucial steps in the process of nucleation and droplet-formation in the gas phase. The coordinate transformations discussed in the present article are equally useful in the study systems of identical particles within classical mechanics, such as in molecular dynamics simulations of gas-phase atomic cluster behaviour.

The generalization of the algorithm to more than two clusters involves some further angular momentum recoupling transformations, but is otherwise straightforward.

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